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Linking Scales in Computations: From Microstructure to Macro-scale Properties

Elementary observations on the averaging of dislocation mechanics: dislocation origin of aspects of anisotropic yield and plastic spin

Amit Acharya[a,*], S. Jonathan Chapman[b]

[a]*Civil & Environmental Engineering, Carnegie Mellon University, Pittsburgh, PA 15213,USA*
[b]*Mathematical Institute, Oxford University, St. Giles 24-29, Oxford OX1 3LB, UK*

Abstract

With a view towards utilization in macroscopic continuum models, an approximation to the root-mean-square of the driving force field on individual dislocations within a "representative volume element" is derived. The plastic flow field of individual dislocations is also similarly averaged. Even under strong simplifying assumptions, non-trivial results on the origin and nature of anisotropic macroscopic yielding, plastic spin, and the plastic flow rule (for single and polycrystalline bodies) are obtained. A particular result is the explicit dependence of the plastic response of a material point of the averaged model on the *presence* of dislocations within it, an effect absent in conventional theories of plastic response (e.g. J_2 plasticity). Also noteworthy is the explicit geometric accounting of the indeterminacy of the slip-plane identity of the screw dislocation that appears to lead to some differences with conventional ideas.

Keywords: dislocation mechanics, macroscopic plasticity, plastic spin, anisotropic yield

1. Introduction

The following questions are of interest in this paper:

- Does there exist any connection between the functional form of the driving force for motion of a single dislocation (with a nonsingular core) and that of a macroscopic yield function for a poly/single crystal?
- Does there exist any connection between the functional form of the plastic strain rate produced by the motion of a single dislocation and that of a macroscopic poly/single crystal?
- Given that the plastic strain rate produced by the motion of a single dislocation is not a symmetric tensor, does this fact provide any clue to the determination of plastic spin of a macroscopic polycrystalline aggregate?

*Corresponding Author
Email addresses: `acharyaamit@cmu.edu` (Amit Acharya), `chapman@maths.ox.ac.uk` (S. Jonathan Chapman)

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The answers to the questions above, *even under severe simplifying assumptions*, lead us to

- an anisotropic polycrystal yield function whose anisotropy is precisely linked to the evolving dislocation structure with the Von-Mises yield function as an isotropic limit, and
- a nonsymmetric plastic flow direction for a macroscopic polycrystal (with the Prandtl-Reuss law as the isotropic limit).

We begin by reviewing a physically rigorous, dislocation mechanics-based framework for plasticity that serves to introduce the basic ingredients and logical thread for the exploration of the questions posed above. The present considerations are limited to the 'small deformation' theory.

The averaging ideas employed herein are elementary and all our results are a direct consequence of essentially the kinematics of the underlying field dislocation mechanics framework. For this reason, the analysis at this level is silent on the important question of size-effects in meso-macro plasticity.

2. (Mesoscale) Field Dislocation Mechanics

The theory uses a continuum description of dislocations based on the concept of Nye's dislocation tensor [1] $\boldsymbol{\alpha}$. Operating on the unit normal field $\boldsymbol{n}$ to a surface A, $\boldsymbol{\alpha}$ delivers the net Burgers vector $\boldsymbol{b}$ of all dislocation lines threading A:

$$\boldsymbol{b} = \int_A \boldsymbol{\alpha}\, \boldsymbol{n}\, da.$$

Nye's definition does not make clear how one might represent a single dislocation by the Nye tensor. For our purposes such a conceptual representation is essential, and we define it as follows. Consider first the situation where any field point $(\boldsymbol{x}, t)$ is occupied by a dislocation segment of a single type (e.g. there are no junctions). The dislocation density at any point and time is then represented as

$$\boldsymbol{\alpha}(\boldsymbol{x}, t) = b\rho(\boldsymbol{x}, t)\, \boldsymbol{m}(\boldsymbol{x}, t) \otimes \boldsymbol{l}(\boldsymbol{x}, t), \tag{1}$$

where b is the magnitude of the Burgers vector, $\boldsymbol{m}(\boldsymbol{x}, t)$ is a unit vector representing the Burgers vector direction of the dislocation segment at $\boldsymbol{x}$ at time t (often one of a collection of slip directions in the material), $\boldsymbol{l}(\boldsymbol{x}, t)$ is a unit vector representing the line direction of the infinitesimal dislocation segment situated at $\boldsymbol{x}$ at time t, and ρ is a real number representing a density (per unit area), defined as follows. Consider a non-singular dislocation at any given time as a disjoint union of a collection of similarly oriented curves (either all closed or all open) that form a solid cylinder called the *core*. The core cylinder can be of non-uniform cross section along its length. By definition, each point of the core can be associated with a unit vector field representing the unit tangent to the curve that passes through it. We denote this unit tangent field as the field $\boldsymbol{l}(\boldsymbol{x})$ within the core. We can now view the core cylinder as a disjoint union of a collection of 2-d, oriented surface patches, each element of which has a well-defined unit normal field associated with it. We now require that on each such surface s with unit normal field $\boldsymbol{n}$ the density field ρ should satisfy the constraint

$$\int_s \rho(\boldsymbol{x})\, \boldsymbol{l}(\boldsymbol{x}) \cdot \boldsymbol{n}(\boldsymbol{x})\, da = 1,$$

and assume that any such density field defines a smooth distribution in the core cylinder. We require that in addition the density field vanish outside the core cylinder. Thus, the density field defined in all of space representing a single dislocation ensures that its strength evaluates to its Burgers vector when tested on any surface s cutting the core:

$$\int_s \boldsymbol{\alpha}(\boldsymbol{x})\, \boldsymbol{n}(\boldsymbol{x})\; da = b\tilde{\boldsymbol{m}},$$

where, in the case of the single dislocation, the field $\boldsymbol{m}$ is spatially uniform and given by $\boldsymbol{m}(\boldsymbol{x}) = \tilde{\boldsymbol{m}}$, the direction of the Burgers vector. Clearly, when junctions/intersections are involved, the dislocation density tensor generally takes the form

$$\boldsymbol{\alpha}(\boldsymbol{x},t) = \sum_{i=1}^{N} b_i \rho_i(\boldsymbol{x},t)\, \boldsymbol{m}_i(\boldsymbol{x},t) \otimes \boldsymbol{l}_i(\boldsymbol{x},t),$$

N being the number of dislocation types involved in the intersection.

Due to lattice incompatibility, $\boldsymbol{U}^p$, the plastic distortion, is not a gradient; it is written as a sum of a gradient and an incompatible part that cannot be expressed as a gradient:

$$\boldsymbol{U}^p = grad\, \boldsymbol{z} - \boldsymbol{\chi}.$$

The incompatible part results from the distribution $\boldsymbol{\alpha}$ through the fundamental geometrical equation of incompatibility

$$curl\, \boldsymbol{U}^p = \boldsymbol{\alpha} \Rightarrow -curl\, \boldsymbol{\chi} = \boldsymbol{\alpha}$$

with the side conditions

$$\begin{aligned} &div\, \boldsymbol{\chi} = \boldsymbol{0} \\ &\boldsymbol{\chi n} = \boldsymbol{0} \ \text{ on the boundary with unit normal } \boldsymbol{n} \end{aligned}$$

to ensure that when $\boldsymbol{\alpha} = 0$ the incompatible part $\boldsymbol{\chi}$ vanishes identically on the body. The compatible part $grad\boldsymbol{z}$ depends upon the history of plastic straining and records the compatible increments of the plastic strain rate produced by the motion of the dislocation density through the equation

$$div\, grad\, \dot{\boldsymbol{z}} = div\, (\boldsymbol{\alpha} \times \boldsymbol{V}).$$

In this model of dislocation mechanics, the total displacement field, $\boldsymbol{u}$, does not represent the actual physical motion of atoms involving topological changes but only a consistent shape change and hence is not required to be discontinuous. However, the stress produced by these topological changes in the lattice is adequately reflected in the theory through the utilization of incompatible elastic/plastic distortions. As usual in continuum plasticity, the elastic distortion (nonsymmetric) is assumed to be the difference of the total displacement gradient and the plastic distortion,

$$\boldsymbol{U}^e := grad\, \boldsymbol{u} - \boldsymbol{U}^p,$$

and the stress is a function of the elastic distortion (in the linear elastic case given by $\boldsymbol{T} = \boldsymbol{C}\boldsymbol{U}^e$) satisfying the equation of equilibrium

$$div\, \boldsymbol{T} = \boldsymbol{0}.$$

Finally, $\boldsymbol{\alpha}$ evolves according to the fundamental conservation law

$$\dot{\boldsymbol{\alpha}} = -curl\, (\boldsymbol{\alpha} \times \boldsymbol{V}^*)$$

where the field $\boldsymbol{V}^*$ at any spatio-temporal location represents the velocity of the infinitesimal dislocation segment at that location. Gathering all equations, the complete theory reads as

$$\begin{aligned} &curl\, \boldsymbol{\chi} = \boldsymbol{\alpha} \\ &div\, \boldsymbol{\chi} = \boldsymbol{0} \\ &div\,(grad\, \dot{\boldsymbol{z}}) = div\,(\boldsymbol{\alpha} \times \boldsymbol{V}^*) \\ &div\,[\boldsymbol{C} : \{grad\, (\boldsymbol{u} - \boldsymbol{z}) + \boldsymbol{\chi}\}] = \boldsymbol{0} \\ &\dot{\boldsymbol{\alpha}} = -curl\,(\boldsymbol{\alpha} \times \boldsymbol{V}^*). \end{aligned} \tag{2}$$

The mechanical dissipation (rate of external working minus the rate of change of stored energy) in the model can be written as

$$D = \int_B \boldsymbol{X}(\boldsymbol{T\alpha}) \cdot \boldsymbol{V}^*\, dv$$

which suggests the maximum-dissipation based driving force for $\boldsymbol{V}^*$ to be $\boldsymbol{X}(\boldsymbol{T\alpha})$ and a linear kinetics-based constitutive assumption for it as

$$\boldsymbol{V}^* = \frac{1}{B}\frac{\boldsymbol{XT}^T\boldsymbol{\alpha}}{|\boldsymbol{\alpha}|}$$

where B is a drag coefficient.

As shown in Section 3.1 below, in order to incorporate the crystallographic constraint that in many circumstances mixed and edge dislocation segments cannot climb, we utilize a slightly different driving force and a consequent velocity law denoted by $\boldsymbol{V}$ in the sequel.

To derive the structure of an averaged theory (Mesoscale Field Dislocation Mechanics, MFDM) corresponding to (2), we adapt a commonly used averaging procedure utilized in the study of multiphase flows (e.g. [2]) for our purposes. For a microscopic field f given as a function of space and time, we define the mesoscopic space-time averaged field $\bar{f}$ as follows:

$$\bar{f}(\boldsymbol{x},t) := \frac{1}{\int_{I(t)}\int_{\Omega(\boldsymbol{x})} w(\boldsymbol{x}-\boldsymbol{x}',t-t')\,d\boldsymbol{x}'dt'}\int_{\Im}\int_{B} w(\boldsymbol{x}-\boldsymbol{x}',t-t')\,f(x',t')\,d\boldsymbol{x}'dt',$$

where B is the body and $\Im$ a sufficiently large interval of time. In the above, $\Omega(\boldsymbol{x})$ is a bounded region within the body around the point $\boldsymbol{x}$ with linear dimension of the order of the spatial resolution of the macroscopic model we seek, and $I(t)$ is a bounded interval in $\Im$ containing t. The averaged field $\bar{f}$ is simply a weighted, space-time, running average of the microscopic field f over regions whose scale is determined by the scale of spatial and temporal resolution of the averaged model one seeks. The weighting function w is non-dimensional, assumed to be smooth in the variables $\boldsymbol{x},\boldsymbol{x}',t,t'$ and, for fixed $\boldsymbol{x}$ and t, have support (i.e. to be non-zero) only in $\Omega(\boldsymbol{x})\times I(t)$ when viewed as a function of $(\boldsymbol{x}',t')$. Applying this operator to the equations in (2), we obtain [3] an *exact* set of equations for the averages given as

$$\begin{aligned}
&curl\,\bar{\boldsymbol{\chi}} = \bar{\boldsymbol{\alpha}}\\
&div\,\bar{\boldsymbol{\chi}} = \boldsymbol{0}\\
&div\,(grad\,\dot{\bar{\boldsymbol{z}}}) = div\left(\bar{\boldsymbol{\alpha}}\times\bar{\boldsymbol{V}} + \boldsymbol{L}^p\right)\\
&\bar{\boldsymbol{U}}^e = grad\,(\bar{\boldsymbol{u}}-\bar{\boldsymbol{z}}) + \bar{\boldsymbol{\chi}}\\
&div\,\bar{\boldsymbol{T}} = \boldsymbol{0}\\
&\dot{\bar{\boldsymbol{\alpha}}} = -curl\left(\bar{\boldsymbol{\alpha}}\times\bar{\boldsymbol{V}} + \boldsymbol{L}^p\right)
\end{aligned}$$

where $\boldsymbol{L}^p$, defined as

$$\boldsymbol{L}^p(\boldsymbol{x},t) := \overline{(\boldsymbol{\alpha}-\bar{\boldsymbol{\alpha}})\times\boldsymbol{V}}(\boldsymbol{x},t) = \overline{\boldsymbol{\alpha}\times\boldsymbol{V}}(\boldsymbol{x},t) - \bar{\boldsymbol{\alpha}}(\boldsymbol{x},t)\times\bar{\boldsymbol{V}}(\boldsymbol{x},t), \tag{3}$$

and $\bar{\boldsymbol{V}}$ are the terms that require closure. Physically, $\boldsymbol{L}^p$ is representative of a portion of the average slip strain rate produced by the 'microscopic' dislocation density; in particular, it can be non-vanishing even when $\bar{\boldsymbol{\alpha}} = \boldsymbol{0}$ and, as such, it is to be physically interpreted as the strain-rate produced by so-called 'statistical dislocations' (SD), as is also indicated by the extreme right-hand side of (3). The variable $\bar{\boldsymbol{V}}$ has the obvious physical meaning of being a space-time average of the pointwise, microscopic dislocation velocity.

The dissipation in MFDM can be written as

$$D = \int_B \left(\boldsymbol{X}\left(\bar{\boldsymbol{T}}\bar{\boldsymbol{\alpha}}\right)\cdot\bar{\boldsymbol{V}} + \bar{\boldsymbol{T}} : \boldsymbol{L}^p\right)dv.$$

Crystalline plasticity is known to be pressure independent for the most part. Non-negative dissipation and pressure independence is ensured in phenomenological MFDM by the choices

$$\boldsymbol{L}^p \text{ is deviatoric and}$$
$$\bar{\boldsymbol{V}} = v\frac{\boldsymbol{d}}{|\boldsymbol{d}|}\ v \geq 0$$
$$\boldsymbol{d} := \boldsymbol{b} - \left(\boldsymbol{b}\cdot\frac{\boldsymbol{a}}{|\boldsymbol{a}|}\right)\frac{\boldsymbol{a}}{|\boldsymbol{a}|},$$
$$\boldsymbol{b} := \boldsymbol{X}\left(\bar{\boldsymbol{T}}'\bar{\alpha}\right)\ ;\ b_i = e_{ijk}\bar{T}'_{jr}\bar{\alpha}_{rk}\ ;\ \boldsymbol{a} := \boldsymbol{X}\left(tr\left(\bar{\boldsymbol{T}}\right)\bar{\alpha}\right)\ ;\ a_i = \left(\frac{1}{3}\bar{T}_{mm}\right)e_{ijk}\bar{\alpha}_{jk}.$$

To understand the choice for the averaged velocity direction $\boldsymbol{d}$, consider the dissipation due to polar dislocation motion, $\boldsymbol{X}\left(\bar{\boldsymbol{T}}\bar{\alpha}\right)\cdot\bar{\boldsymbol{V}}$, and write

$$\boldsymbol{X}\left(\bar{\boldsymbol{T}}\bar{\alpha}\right) = \boldsymbol{b} + \boldsymbol{a}$$

where $\boldsymbol{b}$ is a pressure-independent term, and it makes physical sense to require $\bar{\boldsymbol{V}}$ to be in the direction of $\boldsymbol{b}$. However, this does not guarantee that the dissipation due to polar dislocation motion is independent of pressure and neither that $\boldsymbol{X}\left(\bar{\boldsymbol{T}}\bar{\alpha}\right)\cdot\boldsymbol{b} \geqslant \boldsymbol{0}$; however subtracting the component of $\boldsymbol{b}$ in the direction of $\boldsymbol{a}$ ensures the latter fact:

$$(\boldsymbol{b}+\boldsymbol{a})\cdot\left(\boldsymbol{b} - \left(\boldsymbol{b}\cdot\frac{\boldsymbol{a}}{|\boldsymbol{a}|}\right)\frac{\boldsymbol{a}}{|\boldsymbol{a}|}\right) = \boldsymbol{b}\cdot\boldsymbol{b} - \frac{(\boldsymbol{b}\cdot\boldsymbol{a})^2}{|\boldsymbol{a}|^2} + \boldsymbol{a}\cdot\boldsymbol{b} - \boldsymbol{b}\cdot\boldsymbol{a} = \boldsymbol{b}\cdot\boldsymbol{b} - \left(\boldsymbol{b}\cdot\frac{\boldsymbol{a}}{|\boldsymbol{a}|}\right)^2 \geqslant 0$$

by the Cauchy-Schwarz Inequality (Pythagoras's theorem).

Of course, the primary goal of this paper is to improve/provide guidance on such phenomenological specification for the constitutive definition of the terms $\boldsymbol{L}^p$ and $\bar{\boldsymbol{V}}$. The challenge is formidable as it involves averaging what may be loosely referred to as a nonlinear hyperbolic-elliptic system of equations (when $\boldsymbol{V}$ is assumed to be a given functions of space and time, the evolution equation for $\boldsymbol{\alpha}$ can be shown to be hyperbolic). In the interest of practical tractability, in this paper we attempt an elementary advance towards such constitutive specification by distilling a few algebraic relations pertaining to these averaged quantities under 'mean field' assumptions. In this connection, as defined in (3), the plastic strain rate of the statistical dislocations can be written as

$$\boldsymbol{L}^p := \overline{\boldsymbol{\alpha}\times\boldsymbol{V}} - \bar{\boldsymbol{\alpha}}\times\bar{\boldsymbol{V}},$$

and in the sequel we shall approximate this term by the strain rate that would be produced by the current dislocation distribution under the action of the homogeneous mean field stress:

$$\overline{\left\{\boldsymbol{\alpha}\times\boldsymbol{V} - \bar{\boldsymbol{\alpha}}\times\bar{\boldsymbol{V}}\right\}(\boldsymbol{T})} \approx \overline{\boldsymbol{\alpha}\times\boldsymbol{V}\left(\bar{\boldsymbol{T}}\right)}$$

Clearly, in the cases when $\bar{\boldsymbol{\alpha}} = \boldsymbol{0}$ or $\bar{\boldsymbol{V}} = 0$ in the averaging volume (or $\bar{\boldsymbol{\alpha}}\times\bar{\boldsymbol{V}} = \boldsymbol{0}$), up to the further evaluation at the mean field stress, this is a somewhat justifiable step.

3. Macroscopic Yield Functions and Plastic Strain-Rate Directions

3.1. Polycrystal model, pure edges and mixed dislocations cannot climb

From thermodynamics and maximum dissipation in FDM [4], we have,

$$\boldsymbol{V}^* = \frac{1}{B}\frac{\boldsymbol{X}\boldsymbol{T}^T\boldsymbol{\alpha}}{|\alpha|} = \frac{\boldsymbol{F}^*}{B} \qquad\qquad [B] = \frac{Force.Time}{Area.Length}.$$

Let $p = -\frac{1}{3}(\boldsymbol{T}:\boldsymbol{I})$ and $\boldsymbol{S}$ the stress deviator. Then

$$\boldsymbol{F}^* = \frac{\boldsymbol{X}\boldsymbol{S}^T\boldsymbol{\alpha}}{|\alpha|} + p\frac{\boldsymbol{X}\boldsymbol{\alpha}}{|\alpha|}. \tag{4}$$

Thinking of $\boldsymbol{\alpha}$ at a given space-time location as an elementary dyad of a Burgers vector and a line direction (1), the second term in (4) is part of the driving force that provides a climb force on dislocation segments with a pure edge or mixed character; pure screw dislocation motion is unaffected by the pressure. Thus, if we now assume that dislocations with any edge character cannot climb due to crystallographic constraints, then the relevant part of the driving force is the pressure independent part. However, this still does not mean that the part that is left over, i.e.

$$\frac{\boldsymbol{X}\boldsymbol{S}^T\boldsymbol{\alpha}}{|\boldsymbol{\alpha}|}$$

has no component in the climb direction given by

$$\boldsymbol{X}\boldsymbol{\alpha}$$

(where we note that the climb direction is correctly null in the case of a pure screw). Thus, we *assume that the driving force for dislocation motion encompassing the crystallographic constraint that edges cannot climb* is given by

$$\boldsymbol{F} = \frac{\boldsymbol{XS\alpha}}{|\boldsymbol{\alpha}|} - \left(\frac{\boldsymbol{XS\alpha}}{|\boldsymbol{\alpha}|}\cdot\frac{\boldsymbol{X\alpha}}{|\boldsymbol{X\alpha}|}\right)\frac{\boldsymbol{X\alpha}}{|\boldsymbol{X\alpha}|}. \tag{5}$$

We would now like to consider the "root mean-square of the driving force" on dislocations in the averaging volume:

$$\sqrt{\boldsymbol{F}\cdot\boldsymbol{F}}.$$

With (5) in mind and using the identity

$$\{\boldsymbol{a} - (\boldsymbol{a}\cdot\boldsymbol{b})\,\boldsymbol{b}\}\cdot\{\boldsymbol{a} - (\boldsymbol{a}\cdot\boldsymbol{b})\,\boldsymbol{b}\} = \boldsymbol{a}\cdot\boldsymbol{a} - (\boldsymbol{a}\cdot\boldsymbol{b})^2$$

for $\boldsymbol{a}$ any vector and $\boldsymbol{b}$ a unit vector, we have

$$\boldsymbol{F}\cdot\boldsymbol{F} = \underbrace{\frac{(\boldsymbol{XS\alpha})\cdot(\boldsymbol{XS\alpha})}{(\boldsymbol{\alpha}:\boldsymbol{\alpha})}}_{I} - \underbrace{\frac{(\boldsymbol{XS\alpha}\cdot\boldsymbol{X\alpha})^2}{(\boldsymbol{\alpha}:\boldsymbol{\alpha})(\boldsymbol{X\alpha}\cdot\boldsymbol{X\alpha})}}_{II}$$

Now,

$$|\boldsymbol{\alpha}|^2 I = \varepsilon_{ijk}S_{jr}\alpha_{rk}\varepsilon_{imn}S_{mp}\alpha_{pn} = \left[\delta_{jm}\delta_{kn} - \delta_{jn}\delta_{km}\right]S_{jr}\alpha_{rk}S_{mp}\alpha_{pn}$$
$$= |\boldsymbol{S\alpha}|^2 - \boldsymbol{S}:(\boldsymbol{\alpha S\alpha}) = |\boldsymbol{S\alpha}|^2 - (\boldsymbol{S\alpha}):(\boldsymbol{S\alpha})^T$$

($\boldsymbol{S}$ is symmetric) and

$$|\boldsymbol{\alpha}|^2 II = \frac{\left(\varepsilon_{ijk}S_{jr}\alpha_{rk}\varepsilon_{ips}\alpha_{ps}\right)^2}{|\boldsymbol{X\alpha}|^2} = \frac{\left\{\left[\delta_{jp}\delta_{ks} - \delta_{js}\delta_{kp}\right]S_{jr}\alpha_{rk}\alpha_{ps}\right\}^2}{|\boldsymbol{X\alpha}|^2}$$
$$= \frac{\left(\boldsymbol{S}:\boldsymbol{\alpha\alpha}^T - \boldsymbol{S}:\boldsymbol{\alpha\alpha}\right)^2}{|\boldsymbol{X\alpha}|^2}.$$

Therefore,

$$\boldsymbol{F}\cdot\boldsymbol{F} = \frac{|\boldsymbol{S\alpha}|^2}{|\boldsymbol{\alpha}|^2} - \frac{(\boldsymbol{S\alpha}):(\boldsymbol{S\alpha})^T}{|\boldsymbol{\alpha}|^2} - \frac{\left(\boldsymbol{S}:\boldsymbol{\alpha\alpha}^T\right)^2}{|\boldsymbol{X\alpha}|^2|\boldsymbol{\alpha}|^2} + \frac{2\left(\boldsymbol{S}:\boldsymbol{\alpha\alpha}^T\right)(\boldsymbol{S}:\boldsymbol{\alpha\alpha})}{|\boldsymbol{X\alpha}|^2|\boldsymbol{\alpha}|^2} - \frac{(\boldsymbol{S}:\boldsymbol{\alpha\alpha})^2}{|\boldsymbol{X\alpha}|^2|\boldsymbol{\alpha}|^2}.$$

We now make the *approximation* that the dislocation density at any field point and time may be represented as in (1). *It is important to note that* $\boldsymbol{l}, \boldsymbol{m}$ *vary with time at fixed* $\boldsymbol{x}$ *as dislocations move in the material*. Then

$$|\boldsymbol{\alpha}|^2 = b^2\rho^2 \quad \text{and} \quad \frac{\boldsymbol{\alpha\alpha}^T}{|\boldsymbol{\alpha}|^2} = \boldsymbol{m}\otimes\boldsymbol{m}$$

and

$$\begin{aligned}|X\alpha|^2 &= \varepsilon_{ijk}\alpha_{jk}\varepsilon_{imn}\alpha_{mn} = \left[\delta_{jm}\delta_{kn} - \delta_{jn}\delta_{km}\right]\alpha_{jk}\alpha_{mn}\\ &= \alpha_{mn}\alpha_{mn} - \alpha_{nk}\alpha_{kn} = b^2\rho^2 m_n l_k m_k l_n\\ &= b^2\rho^2\left\{1-(\boldsymbol{l}\cdot\boldsymbol{m})^2\right\}.\end{aligned}$$

So

$$\begin{aligned}&(\boldsymbol{S}\alpha):(\boldsymbol{S}\alpha) = S_{mr}\alpha_{rn}\alpha_{pn}S_{mp}b^2\rho^2\\ &\Rightarrow \frac{|\boldsymbol{S}\alpha|^2}{|\alpha|^2} = \boldsymbol{S}^T\boldsymbol{S}:(\boldsymbol{m}\otimes\boldsymbol{m});\end{aligned}$$

$$\begin{aligned}&(\boldsymbol{S}\alpha):(\boldsymbol{S}\alpha)^T = S_{nr}\alpha_{rm}\alpha_{pn}S_{mp}b^2\rho^2 = S_{rn}S_{pm}m_r l_n m_p l_m b^2\rho^2\\ &\Rightarrow -\frac{(\boldsymbol{S}\alpha):(\boldsymbol{S}\alpha)^T}{|\alpha|^2} = -\boldsymbol{S}:[(\boldsymbol{m}\otimes\boldsymbol{l})\otimes(\boldsymbol{m}\otimes\boldsymbol{l})]:\boldsymbol{S};\end{aligned}$$

$$\begin{aligned}&\left(\boldsymbol{S}:\alpha\alpha^T\right)^2 = \left(S_{pr}\alpha_{rs}\alpha_{ps}\right)^2 = \left(S_{pr}m_r m_p b^2\rho^2\right)^2\\ &\Rightarrow -\frac{\left(\boldsymbol{S}:\alpha\alpha^T\right)^2}{|X\alpha|^2|\alpha|^2} = -\frac{\boldsymbol{S}:[(\boldsymbol{m}\otimes\boldsymbol{m})\otimes(\boldsymbol{m}\otimes\boldsymbol{m})]:\boldsymbol{S}}{\left(1-(\boldsymbol{l}\cdot\boldsymbol{m})^2\right)};\end{aligned}$$

$$\begin{aligned}&\left(\boldsymbol{S}:\alpha\alpha^T\right) = \boldsymbol{S}:(\boldsymbol{m}\otimes\boldsymbol{m})\,b^2\rho^2\\ &(\boldsymbol{S}:\alpha\alpha) = \boldsymbol{S}:(\boldsymbol{m}\otimes\boldsymbol{l})\,b^2\rho^2\,(\boldsymbol{l}\cdot\boldsymbol{m})\\ &\Rightarrow \frac{2\left(\boldsymbol{S}:\alpha\alpha^T\right)(\boldsymbol{S}:\alpha\alpha)}{|X\alpha|^2|\alpha|^2} = 2\frac{\boldsymbol{S}:[(\boldsymbol{m}\otimes\boldsymbol{m})\otimes(\boldsymbol{m}\otimes\boldsymbol{l})]:\boldsymbol{S}\,(\boldsymbol{l}\cdot\boldsymbol{m})}{\left(1-(\boldsymbol{l}\cdot\boldsymbol{m})^2\right)};\end{aligned}$$

$$\begin{aligned}&(\boldsymbol{S}:\alpha\alpha) = \boldsymbol{S}:(\boldsymbol{m}\otimes\boldsymbol{l})\,(\boldsymbol{l}\cdot\boldsymbol{m})\,b^2\rho^2\\ &\Rightarrow -\frac{(\boldsymbol{S}:\alpha\alpha)^2}{|X\alpha|^2|\alpha|^2} = -\frac{\boldsymbol{S}:[(\boldsymbol{m}\otimes\boldsymbol{l})\otimes(\boldsymbol{m}\otimes\boldsymbol{l})]:\boldsymbol{S}(\boldsymbol{l}\cdot\boldsymbol{m})^2}{\left(1-(\boldsymbol{l}\cdot\boldsymbol{m})^2\right)},\end{aligned}$$

and

$$\begin{aligned}\boldsymbol{F}\cdot\boldsymbol{F} &= \boldsymbol{S}\boldsymbol{S}^T:(\boldsymbol{m}\otimes\boldsymbol{m})\\ &-\boldsymbol{S}:[(\boldsymbol{m}\otimes\boldsymbol{l})\otimes(\boldsymbol{m}\otimes\boldsymbol{l})]:\boldsymbol{S}\\ &+\boldsymbol{S}:\left[\frac{1}{\left(1-(\boldsymbol{l}\cdot\boldsymbol{m})^2\right)}\left\{\begin{array}{l}-(\boldsymbol{m}\otimes\boldsymbol{m})\otimes(\boldsymbol{m}\otimes\boldsymbol{m})\\ +2\,(\boldsymbol{m}\otimes\boldsymbol{m})\otimes(\boldsymbol{m}\otimes\boldsymbol{l})\,(\boldsymbol{l}\cdot\boldsymbol{m})\\ -(\boldsymbol{m}\otimes\boldsymbol{l})\otimes(\boldsymbol{m}\otimes\boldsymbol{l})\,(\boldsymbol{l}\cdot\boldsymbol{m})^2\end{array}\right\}\right]:\boldsymbol{S}.\end{aligned} \tag{6}$$

To check if (6) corresponds to the usual notion of driving stress components for motion of dislocations lying on specific slip planes, let $\boldsymbol{n}, \boldsymbol{q}$ be *any* two orthonormal directions such that along with $\boldsymbol{m}$ (slip direction) they form an orthonormal triad. In particular, but not necessarily, $\boldsymbol{n}, \boldsymbol{q}$ could be chosen to be a slip plane normal and $\boldsymbol{q} = \boldsymbol{m}\times\boldsymbol{n}$ respectively. Then

$$\begin{aligned}\boldsymbol{S}\boldsymbol{S}^T &= [(\boldsymbol{S}\boldsymbol{m})\otimes\boldsymbol{m} + (\boldsymbol{S}\boldsymbol{n})\otimes\boldsymbol{n} + (\boldsymbol{S}\boldsymbol{q})\otimes\boldsymbol{q}]\,[\boldsymbol{m}\otimes(\boldsymbol{S}\boldsymbol{m}) + \boldsymbol{n}\otimes(\boldsymbol{S}\boldsymbol{n}) + \boldsymbol{q}\otimes(\boldsymbol{S}\boldsymbol{q})]\\ &= [(\boldsymbol{S}\boldsymbol{m})\otimes(\boldsymbol{S}\boldsymbol{m}) + (\boldsymbol{S}\boldsymbol{n})\otimes(\boldsymbol{S}\boldsymbol{n}) + (\boldsymbol{S}\boldsymbol{q})\otimes(\boldsymbol{S}\boldsymbol{q})],\end{aligned}$$

so that

$$\begin{aligned}&\boldsymbol{S}\boldsymbol{S}^T:(\boldsymbol{m}\otimes\boldsymbol{m}) = (S_{mm})^2 + \tau^2 + \left(S_{mq}\right)^2 \text{ (no sum)}\\ &S_{mm} := \boldsymbol{m}\cdot\boldsymbol{S}\boldsymbol{m} \quad;\quad \tau = \boldsymbol{m}\cdot\boldsymbol{S}\boldsymbol{n} \quad;\quad S_{mq} = \boldsymbol{m}\cdot\boldsymbol{S}\boldsymbol{q}.\end{aligned}$$

In the case of a pure edge dislocation segment ($\boldsymbol{q} = \boldsymbol{l}$ and $\boldsymbol{l}\cdot\boldsymbol{m} = 0$) lying in the slip plane normal to $\boldsymbol{n}$, the magnitude of the driving stress is the resolved shear stress on the slip plane:

$$\sqrt{\boldsymbol{F}\cdot\boldsymbol{F}} = |\tau| \quad \text{(pure edge)}. \tag{7}$$

In the case of a pure screw segment ($\boldsymbol{m} = \boldsymbol{l}$) the magnitude of the driving force is

$$\sqrt{\boldsymbol{F}\cdot\boldsymbol{F}} = \sqrt{\tau^2 + \left(S_{mq}\right)^2} \qquad \text{(pure screw)} \tag{8}$$

regardless of the orientation of the orthogonal vectors $\boldsymbol{n}, \boldsymbol{q}$ *perpendicular to* $\boldsymbol{m}$, since a pure screw segment cannot be assigned a slip plane. To consider the case of the mixed dislocation segment lying in the slip plane it is best to revert to the form (5) and note that $\boldsymbol{S}$ is symmetric so that

$$\frac{\boldsymbol{X}\boldsymbol{S}\boldsymbol{\alpha}}{|\boldsymbol{\alpha}|} = \boldsymbol{X}\boldsymbol{S}\left(\boldsymbol{m}\otimes\boldsymbol{l}\right) \quad ; \quad \boldsymbol{S} = \boldsymbol{S}^T = \boldsymbol{m}\otimes(\boldsymbol{S}\boldsymbol{m}) + \boldsymbol{q}\otimes(\boldsymbol{S}\boldsymbol{q}) + \boldsymbol{n}\otimes(\boldsymbol{S}\boldsymbol{n}) \quad ; \quad \boldsymbol{l} = l_e\boldsymbol{q} + l_s\boldsymbol{m}$$

which further implies

$$\frac{\boldsymbol{X}\boldsymbol{S}\boldsymbol{\alpha}}{|\boldsymbol{\alpha}|} = \boldsymbol{X}\boldsymbol{S}\left(\boldsymbol{m}\otimes\boldsymbol{l}\right) = S_{mm}l_e\boldsymbol{m}\times\boldsymbol{q} + S_{mq}l_s\boldsymbol{q}\times\boldsymbol{m} + \tau\boldsymbol{n}\times\boldsymbol{l} \quad ; \quad \boldsymbol{X}\boldsymbol{\alpha}//\boldsymbol{m}\times\boldsymbol{q},$$

so that the driving stress in the case of a mixed segment is again just the resolved shear stress:

$$\sqrt{\boldsymbol{F}\cdot\boldsymbol{F}} = |\tau| \qquad \text{(mixed).} \tag{9}$$

Let us now make the drastic assumption that $\boldsymbol{S}(\boldsymbol{x}', t') = \bar{\boldsymbol{S}}(\boldsymbol{x}, t)$ where the spatial averaging volume is assumed to be over many grains. Then

$$\begin{aligned}\overline{\boldsymbol{F}\cdot\boldsymbol{F}} &\approx \bar{\boldsymbol{S}}\bar{\boldsymbol{S}}^T : \overline{\boldsymbol{m}\otimes\boldsymbol{m}} \\ &- \bar{\boldsymbol{S}} : \overline{\left[(\boldsymbol{m}\otimes\boldsymbol{l})\otimes(\boldsymbol{m}\otimes\boldsymbol{l})\right]} : \bar{\boldsymbol{S}} \\ &+ \bar{\boldsymbol{S}} : \overline{\left[\frac{1}{\left(1-(\boldsymbol{l}\cdot\boldsymbol{m})^2\right)}\begin{Bmatrix} -(\boldsymbol{m}\otimes\boldsymbol{m})\otimes(\boldsymbol{m}\otimes\boldsymbol{m}) \\ +2\,(\boldsymbol{m}\otimes\boldsymbol{m})\otimes(\boldsymbol{m}\otimes\boldsymbol{l})\,(\boldsymbol{l}\cdot\boldsymbol{m}) \\ -(\boldsymbol{m}\otimes\boldsymbol{l})\otimes(\boldsymbol{m}\otimes\boldsymbol{l})\,(\boldsymbol{l}\cdot\boldsymbol{m})^2 \end{Bmatrix}\right]} : \bar{\boldsymbol{S}} \\ &=: \varphi^2\left(\bar{\boldsymbol{S}}\right).\end{aligned} \tag{10}$$

If we now postulate $\varphi\left(\bar{\boldsymbol{S}}\right)$ as a yield function for the polycrystal, we see that we have arrived at a generally *anisotropic* yield function

1. whose anisotropy is precisely linked to the averaged evolution of the dislocation microstructure and is affected by the *availability* and *type* of dislocation segments in the averaging volume (an effect absent in the conventional theory where the dependence of anisotropy is only on the lattice reorientation); the (evolution of the) fourth order structure tensors of anisotropy can in principle be approximately defined, at least along specific applied loading paths, from Discrete Dislocation simulations for polycrystalline assemblies;
2. which accounts for driving forces on screw dislocations unambiguously thus yielding a difference in result from what would have been obtained from the (closest) classical crystal plasticity paradigm by averaging only the resolved shear stress over the possible slip system orientations in the averaging volume;
3. for which (10) is an invariant representation independent of the arbitrary choice of the directions $\boldsymbol{q}, \boldsymbol{n}$ used to define the "slip system driving stress components," ;
4. that can allow purely elastic response, independent of stress magnitude, in case the averaging volume does not contain any dislocations.

To elaborate on the remark above related to the availability of dislocations, consider the case when there are only mixed and pure edge segments within the averaging volume; then, the exercise leading to (7-9) implies that the averaging problem may well be thought of as averaging the resolved shear stress on available slip systems within the averaging volume. In conventional plasticity, this is a problem that only involves knowing the microscopic stress field and the crystallography of the material; from the dislocation point of view, it is a question of knowing the microscopic stress field, the crystallography of the material, as well as the knowledge of the microscopic dislocation density field. Thus the evolution of anisotropy depends not only on stress evolution and lattice reorientation, but also on the evolution of the dislocation microstructure. We finally note that (7-9) imply that (10) may also be written in the form

$$\overline{\boldsymbol{F}\cdot\boldsymbol{F}} \approx \bar{\boldsymbol{S}} : \overline{\left[(\boldsymbol{m}\otimes\boldsymbol{n})\otimes(\boldsymbol{m}\otimes\boldsymbol{n}) + \chi_{ps}(\boldsymbol{m}\otimes\boldsymbol{q})\otimes(\boldsymbol{m}\otimes\boldsymbol{q})\right]} : \bar{\boldsymbol{S}} \tag{11}$$

where χ_{ps} is the characteristic function of pure-screw dislocation segments within the space-time averaging volume;

$$\chi_{ps}(\boldsymbol{x},t) = \begin{cases} 1 \text{ if } |\boldsymbol{m}(\boldsymbol{x},t)\cdot\boldsymbol{l}(\boldsymbol{x},t)| = 1 \\ 0 \text{ otherwise.} \end{cases} \tag{12}$$

In case the fourth-order averaged orientation tensor appearing in (11) is assumed to be isotropic, then (due to the fact that $\boldsymbol{S}$ is deviatoric),

$$\sqrt{\overline{\boldsymbol{F}\cdot\boldsymbol{F}}} \approx \sqrt{a\,\bar{\boldsymbol{S}}:\bar{\boldsymbol{S}}}$$

for some scalar a, taking on a form quite close to the yield function of conventional Von-Mises J_2 plasticity theory. It is interesting to note that if the averaged orientation tensor is isotropic for one choice of the $\boldsymbol{n},\boldsymbol{q}$ fields (up to being point-wise orthogonal to the $\boldsymbol{m}$ field) then it is isotropic for any other choice satisfying the same constraint, a fact that is not obvious from (11) but is true because of the equivalence between (11) and (10).

We now focus on the direction of plastic flow. The microscopic plastic strain rate is given as

$$\boldsymbol{\alpha} \times \boldsymbol{V} = \boldsymbol{\alpha} \times \frac{1}{B}\boldsymbol{F}, \tag{13}$$

where $\boldsymbol{F}$ is given by (5). To evaluate (13) consider first

$$\begin{aligned}
\left(\boldsymbol{\alpha} \times \frac{\boldsymbol{X}(\boldsymbol{S\alpha})}{|\boldsymbol{\alpha}|}\right)_{qp} &= \frac{\varepsilon_{ijk}S_{jr}\alpha_{rk}}{|\boldsymbol{\alpha}|}\varepsilon_{pmi}\alpha_{qm} = \left[\delta_{pj}\delta_{mk} - \delta_{pk}\delta_{mj}\right]\frac{\alpha_{qm}S_{jr}\alpha_{rk}}{|\boldsymbol{\alpha}|} \\
&= \frac{1}{|\boldsymbol{\alpha}|}\left[\alpha_{qk}S_{pr}\alpha_{rk} - \alpha_{qj}S_{jr}\alpha_{rk}\right] \\
\Rightarrow \left(\boldsymbol{\alpha} \times \frac{\boldsymbol{X}(\boldsymbol{S\alpha})}{|\boldsymbol{\alpha}|}\right) &= \frac{1}{|\boldsymbol{\alpha}|}\left[\left(\boldsymbol{\alpha\alpha}^T\right)\boldsymbol{S}^T - \boldsymbol{\alpha S \alpha}\right],
\end{aligned}$$

and then

$$\begin{aligned}
\left(\boldsymbol{\alpha} \times \frac{\boldsymbol{X\alpha}}{|\boldsymbol{X\alpha}|}\right)_{qp} &= \frac{1}{|\boldsymbol{X\alpha}|}\varepsilon_{pmi}\alpha_{qm}\varepsilon_{ijk}\alpha_{jk} = \frac{1}{|\boldsymbol{X\alpha}|}\left[\delta_{pj}\delta_{mk} - \delta_{pk}\delta_{mj}\right]\alpha_{qm}\alpha_{jk} = \frac{1}{|\boldsymbol{X\alpha}|}\left[\alpha_{qk}\alpha_{pk} - \alpha_{qj}\alpha_{jp}\right] \\
\Rightarrow \left(\boldsymbol{\alpha} \times \frac{\boldsymbol{X\alpha}}{|\boldsymbol{X\alpha}|}\right) &= \frac{1}{|\boldsymbol{X\alpha}|}\left[\boldsymbol{\alpha\alpha}^T - \boldsymbol{\alpha\alpha}\right].
\end{aligned}$$

Therefore

$$\begin{aligned}
\boldsymbol{\alpha} \times \boldsymbol{V} &= \frac{1}{B}\boldsymbol{\alpha} \times \frac{\boldsymbol{X}(\boldsymbol{S\alpha})}{|\boldsymbol{\alpha}|} - \frac{1}{B}\boldsymbol{\alpha} \times \left(\frac{\boldsymbol{XS\alpha}}{|\boldsymbol{\alpha}|}\cdot\frac{\boldsymbol{X\alpha}}{|\boldsymbol{X\alpha}|}\right)\frac{\boldsymbol{X\alpha}}{|\boldsymbol{X\alpha}|} \\
&= \frac{|\boldsymbol{\alpha}|}{B}\left[\frac{\left(\boldsymbol{\alpha\alpha}^T\right)\boldsymbol{S}}{|\boldsymbol{\alpha}|^2} - \frac{\boldsymbol{\alpha S\alpha}}{|\boldsymbol{\alpha}|^2} - \frac{\left(\boldsymbol{S}:\boldsymbol{\alpha\alpha}^T - \boldsymbol{S}:\boldsymbol{\alpha\alpha}\right)}{|\boldsymbol{\alpha}|^2|\boldsymbol{X\alpha}|^2}\left(\boldsymbol{\alpha\alpha}^T - \boldsymbol{\alpha\alpha}\right)\right] \\
&= \frac{|\boldsymbol{\alpha}|}{B}\left[\begin{array}{l} \dfrac{\left(\boldsymbol{\alpha\alpha}^T\right)\boldsymbol{S}}{|\boldsymbol{\alpha}|^2} - \dfrac{\boldsymbol{\alpha S\alpha}}{|\boldsymbol{\alpha}|^2} - \dfrac{\left(\boldsymbol{\alpha\alpha}^T\otimes\boldsymbol{\alpha\alpha}^T\right):\boldsymbol{S}}{|\boldsymbol{\alpha}|^2|\boldsymbol{X\alpha}|^2} + \dfrac{\left(\boldsymbol{\alpha\alpha}\otimes\boldsymbol{\alpha\alpha}^T\right):\boldsymbol{S}}{|\boldsymbol{\alpha}|^2|\boldsymbol{X\alpha}|^2} \\ + \dfrac{\left(\boldsymbol{\alpha\alpha}^T\otimes\boldsymbol{\alpha\alpha}\right):\boldsymbol{S}}{|\boldsymbol{\alpha}|^2|\boldsymbol{X\alpha}|^2} - \dfrac{\left(\boldsymbol{\alpha\alpha}\otimes\boldsymbol{\alpha\alpha}\right):\boldsymbol{S}}{|\boldsymbol{\alpha}|^2|\boldsymbol{X\alpha}|^2} \end{array}\right].
\end{aligned}$$

Define by $\boldsymbol{P}$ the tensor

$$\boldsymbol{P} := \boldsymbol{m}\otimes\boldsymbol{m}\bar{\boldsymbol{S}} - \left[(\boldsymbol{m}\otimes\boldsymbol{l})\otimes(\boldsymbol{m}\otimes\boldsymbol{l})\right] : \bar{\boldsymbol{S}} + \left[\frac{1}{\left(1-(\boldsymbol{l}\cdot\boldsymbol{m})^2\right)}\left\{\begin{array}{l} -(\boldsymbol{m}\otimes\boldsymbol{m})\otimes(\boldsymbol{m}\otimes\boldsymbol{m}) \\ +(\boldsymbol{m}\otimes\boldsymbol{l})\otimes(\boldsymbol{m}\otimes\boldsymbol{m})(\boldsymbol{l}\cdot\boldsymbol{m}) \\ +(\boldsymbol{m}\otimes\boldsymbol{m})\otimes(\boldsymbol{m}\otimes\boldsymbol{l})(\boldsymbol{l}\cdot\boldsymbol{m}) \\ -(\boldsymbol{m}\otimes\boldsymbol{l})\otimes(\boldsymbol{m}\otimes\boldsymbol{l})(\boldsymbol{l}\cdot\boldsymbol{m})^2 \end{array}\right\}\right] : \bar{\boldsymbol{S}}. \tag{14}$$

Making the 'mean-field' assumption on stress as in the case of the yield function, we have

$$\overline{\boldsymbol{\alpha}\times\boldsymbol{V}\left(\bar{\boldsymbol{S}}\right)} = \overline{\left\{\left(\overline{\frac{|\alpha|}{B}}\right)+\left(\frac{|\alpha|}{B}-\left(\overline{\frac{|\alpha|}{B}}\right)\right)\right\}\boldsymbol{P}} = \left(\overline{\frac{|\alpha|}{B}}\right)\bar{\boldsymbol{P}} + \overline{\left(\frac{|\alpha|}{B}-\left(\overline{\frac{|\alpha|}{B}}\right)\right)\boldsymbol{P}}.$$

Recalling the definition and assumption

$$\boldsymbol{L}^p := \overline{\left\{\boldsymbol{\alpha}\times\boldsymbol{V}-\bar{\boldsymbol{\alpha}}\times\bar{\boldsymbol{V}}\right\}(\boldsymbol{S})} \approx \overline{\boldsymbol{\alpha}\times\boldsymbol{V}\left(\bar{\boldsymbol{S}}\right)}$$

and defining

$$\boldsymbol{D}^p := \left(\overline{\frac{|\alpha|}{B}}\right)\bar{\boldsymbol{P}}_{sym} \qquad ; \qquad \boldsymbol{\omega}^p := \left(\overline{\frac{|\alpha|}{B}}\right)\bar{\boldsymbol{P}}_{skw}$$

we have

$$\boldsymbol{L}^p \approx \boldsymbol{D}^p + \boldsymbol{\omega}^p + \overline{\left(\frac{|\alpha|}{B}-\left(\overline{\frac{|\alpha|}{B}}\right)\right)\boldsymbol{P}}.$$

We would now like to explore implications of plastic flow and spin implied by the model of a polycrystal characterized by $\varphi(\boldsymbol{S})$ as the yield function and $\boldsymbol{D}^p + \boldsymbol{\omega}^p$ as the plastic flow.

With reference to (10), consider the function

$$\varphi^2(\boldsymbol{A}) = I + II + III + IV + V$$

of a symmetric tensor, where the terms on the right-hand-side correspond to the five additive terms defining the function φ^2 in (10).

$$\begin{aligned}
& I = \overline{\boldsymbol{A}\boldsymbol{A}^T : \overline{\boldsymbol{m}\otimes\boldsymbol{m}}} = \overline{A_{ip}A_{jp}m_im_j} \\
& \frac{\partial I}{\partial A_{rq}} = \delta_{ir}\delta_{pq}A_{jp}m_im_j + A_{ip}\delta_{jr}\delta_{pq}m_im_j = m_rA_{jq}m_j + A_{iq}m_im_r = 2m_jA_{jq}m_r \\
& \frac{\partial\,()}{\partial A_{qr}} = 2m_jA_{jr}m_q \text{ but } \frac{\partial\,()}{\partial A_{rq}} = \frac{\partial\,()}{\partial A_{qr}} \\
& \therefore \frac{\partial I}{\partial \bar{S}_{rq}} = \overline{m_j\bar{S}_{jq}m_r + m_j\bar{S}_{jr}m_q} \\
& \Rightarrow \frac{\partial I}{\partial\bar{\boldsymbol{S}}} = \bar{\boldsymbol{S}}\,\overline{\boldsymbol{m}\otimes\boldsymbol{m}} + \overline{\boldsymbol{m}\otimes\boldsymbol{m}}\,\bar{\boldsymbol{S}}.
\end{aligned}$$

Next

$$\begin{aligned}
& II = -\overline{A : (m\otimes l)\otimes(m\otimes l) : A} \\
& \frac{\partial II}{\partial A_{rq}} = -m_rl_q\,(m\otimes l) : A - A : (m\otimes l)\,m_rl_q = -2m_rl_q\,(m\otimes l) : A \\
& \frac{1}{2}\left(\frac{\partial II}{\partial A_{rq}} + \frac{\partial II}{\partial A_{qr}}\right) = \frac{\partial II}{\partial A_{rq}} \\
& \therefore \frac{\partial II}{\partial\bar{\boldsymbol{S}}} = -\overline{\{(\boldsymbol{m}\otimes\boldsymbol{l})+(\boldsymbol{l}\otimes\boldsymbol{m})\}\otimes(\boldsymbol{m}\otimes\boldsymbol{l})} : \bar{\boldsymbol{S}}.
\end{aligned}$$

Similarly

$$\frac{\partial III}{\partial \bar{S}} = -2\,\frac{1}{\left(1-(\boldsymbol{l}\cdot\boldsymbol{m})^2\right)}\,\overline{(\boldsymbol{m}\otimes\boldsymbol{m})\otimes(\boldsymbol{m}\otimes\boldsymbol{m})}:\bar{\boldsymbol{S}}$$

$$\frac{\partial IV}{\partial \bar{S}} = 2\,\overline{\frac{(\boldsymbol{l}\cdot\boldsymbol{m})}{\left(1-(\boldsymbol{l}\cdot\boldsymbol{m})^2\right)}\,[(\boldsymbol{m}\otimes\boldsymbol{m})\otimes(\boldsymbol{m}\otimes\boldsymbol{l})]}:\bar{\boldsymbol{S}} + \overline{\frac{(\boldsymbol{l}\cdot\boldsymbol{m})}{\left(1-(\boldsymbol{l}\cdot\boldsymbol{m})^2\right)}\,[\{(\boldsymbol{m}\otimes\boldsymbol{l})+(\boldsymbol{l}\otimes\boldsymbol{m})\}\otimes(\boldsymbol{m}\otimes\boldsymbol{m})]}:\bar{\boldsymbol{S}}$$

$$\frac{\partial V}{\partial \bar{S}} = -\,\overline{\frac{(\boldsymbol{l}\cdot\boldsymbol{m})^2}{\left(1-(\boldsymbol{l}\cdot\boldsymbol{m})^2\right)}\,\{(\boldsymbol{m}\otimes\boldsymbol{l})+(\boldsymbol{l}\otimes\boldsymbol{m})\}\otimes(\boldsymbol{m}\otimes\boldsymbol{l})}:\bar{\boldsymbol{S}}$$

Therefore

$$\bar{\boldsymbol{P}}_{sym} = \frac{1}{2}\frac{\partial\varphi^2}{\partial\bar{\boldsymbol{S}}} \quad\Rightarrow\quad \boxed{\boldsymbol{D}^p // \frac{\partial\varphi}{\partial\bar{\boldsymbol{S}}}}. \tag{15}$$

Thus, if we consider a model of polycrystal response whose plastic flow is governed by

$$\boldsymbol{L}^p_{red} := \boldsymbol{D}^p + \boldsymbol{\omega}^p = \overline{\left(\frac{|\alpha|}{B}\right)}\,\bar{\boldsymbol{P}}$$

and the yield function by

$$\varphi\left(\bar{\boldsymbol{S}}\right),$$

then (15) implies *associated flow* in the model along with *plastic spin* given by

$$\boldsymbol{\omega}^p := \overline{\left(\frac{|\alpha|}{B}\right)}\,\bar{\boldsymbol{P}}_{skw} = \frac{\dot{\gamma}}{|\bar{\boldsymbol{S}}|}\left\{\begin{array}{l} \left[\overline{\boldsymbol{m}\otimes\boldsymbol{m}}\,\bar{\boldsymbol{S}} - \bar{\boldsymbol{S}}\,\overline{\boldsymbol{m}\otimes\boldsymbol{m}}\right] - \overline{[\{(\boldsymbol{m}\otimes\boldsymbol{l})-(\boldsymbol{l}\otimes\boldsymbol{m})\}\otimes(\boldsymbol{m}\otimes\boldsymbol{l})]}:\bar{\boldsymbol{S}} \\ +\left[\overline{\frac{(\boldsymbol{l}\cdot\boldsymbol{m})\{(\boldsymbol{m}\otimes\boldsymbol{l})-(\boldsymbol{l}\otimes\boldsymbol{m})\}}{\left(1-(\boldsymbol{l}\cdot\boldsymbol{m})^2\right)}\otimes\{(\boldsymbol{m}\otimes\boldsymbol{m})-(\boldsymbol{l}\cdot\boldsymbol{m})(\boldsymbol{m}\otimes\boldsymbol{l})\}}\right]:\bar{\boldsymbol{S}} \end{array}\right\}$$

$$\dot{\gamma} := \frac{1}{2}\overline{\left(\frac{|\alpha|}{B}\right)}\,|\bar{\boldsymbol{S}}|.$$

The *plastic strain rate* is given by

$$\boldsymbol{D}^p := \overline{\left(\frac{|\alpha|}{B}\right)}\,\bar{\boldsymbol{P}}_{sym} = \frac{\dot{\gamma}}{|\bar{\boldsymbol{S}}|}\left\{\begin{array}{l} \bar{\boldsymbol{S}}\,\overline{\boldsymbol{m}\otimes\boldsymbol{m}} + \overline{\boldsymbol{m}\otimes\boldsymbol{m}}\,\bar{\boldsymbol{S}} - \overline{\{(\boldsymbol{m}\otimes\boldsymbol{l})+(\boldsymbol{l}\otimes\boldsymbol{m})\}\otimes(\boldsymbol{m}\otimes\boldsymbol{l})}:\bar{\boldsymbol{S}} \\ -\,2\,\frac{1}{\left(1-(\boldsymbol{l}\cdot\boldsymbol{m})^2\right)}\,\overline{(\boldsymbol{m}\otimes\boldsymbol{m})\otimes(\boldsymbol{m}\otimes\boldsymbol{m})}:\bar{\boldsymbol{S}} \\ +\,\overline{\frac{(\boldsymbol{l}\cdot\boldsymbol{m})}{\left(1-(\boldsymbol{l}\cdot\boldsymbol{m})^2\right)}\left(\begin{array}{l} 2\,[(\boldsymbol{m}\otimes\boldsymbol{m})\otimes(\boldsymbol{m}\otimes\boldsymbol{l})] \\ +\,[\{(\boldsymbol{m}\otimes\boldsymbol{l})+(\boldsymbol{l}\otimes\boldsymbol{m})\}\otimes(\boldsymbol{m}\otimes\boldsymbol{m})] \end{array}\right)}:\bar{\boldsymbol{S}} \\ -\,\overline{\frac{(\boldsymbol{l}\cdot\boldsymbol{m})^2}{\left(1-(\boldsymbol{l}\cdot\boldsymbol{m})^2\right)}\,\{(\boldsymbol{m}\otimes\boldsymbol{l})+(\boldsymbol{l}\otimes\boldsymbol{m})\}\otimes(\boldsymbol{m}\otimes\boldsymbol{l})}:\bar{\boldsymbol{S}} \end{array}\right\}.$$

The considerations here do not define the evolution of

- the yield threshold,
- the structure tensors defining the plastic flow direction (and consequently the yield function due to associative flow), and

- the scalar plastic strain rate function.

However, the explicit formulae above may be expected to help in the characterization of the evolution of these response functions from microscopic simulation techniques like Discrete Dislocation Dynamics. A parameter of the dependence of the yield threshold may be expected to be on the fluctuation term defined by

$$\overline{\boldsymbol{F}(\boldsymbol{S}) \cdot \boldsymbol{F}(\boldsymbol{S})} - \varphi^2\left(\bar{\boldsymbol{S}}\right)$$

that depends upon second and higher moments of the stress tensor field over the space-time averaging volume.

3.2. Single crystal model, pure edge and mixed dislocations cannot climb

We distinguish between the single crystal and polycrystal cases by thinking about averaging over smaller spatial regions (i.e. within a single crystal) and, in keeping with the structure of conventional single crystal plasticity [5, 6, 7], we assume that the threshold behavior is different for different slip systems so that we consider averages separately for each slip system. However, since pure screw segments cannot be assigned any particular slip system, we consider averages of the behavior of such segments simply over the space-time domain $I(t) \times \Omega(\boldsymbol{x})$ (which is now encompassed within a single crystal).

Following standard practice, let us characterize the κ^{th} slip system by the slip direction unit vector $\boldsymbol{m}^\kappa$ and the slip plane unit normal $\boldsymbol{n}^\kappa$. Let the characteristic function within the averaging region of non pure-screw segments on the system κ be denoted by χ^κ_{ns},

$$\chi^\kappa_{ns}(\boldsymbol{x}, t) = \begin{cases} 1 \text{ if } |\boldsymbol{m}^\kappa \cdot \boldsymbol{l}(\boldsymbol{x}, t)| \neq 1 \text{ and } \boldsymbol{l}(\boldsymbol{x}, t) \cdot \boldsymbol{n}^\kappa = 0 \text{ and } |\boldsymbol{l}(\boldsymbol{x}, t)| \neq 0 \\ 0 \text{ otherwise.} \end{cases}$$

The characteristic function for pure-screws is denoted by χ_{ps} (12). Denote the driving force on non pure-screw segments on slip system κ as $\boldsymbol{F}^\kappa_{ns}$ and the resolved shear stress on the system as τ^κ. Let the driving stress on the pure screw segments be $\boldsymbol{F}_{ps}$. Following the considerations leading up to (7) and (9), it is clear that

$$\boldsymbol{F}^\kappa_{ns} \cdot \boldsymbol{F}^\kappa_{ns} = \chi_{ns}(\tau^\kappa)^2.$$

Denoting the stress dependence of the resolved shear stress as $\tau^\kappa(\boldsymbol{S}) := \boldsymbol{m}^\kappa \cdot \boldsymbol{S}\boldsymbol{n}^\kappa$, it is natural to define the yield function, $\varphi^\kappa\left(\bar{\boldsymbol{S}}\right)$, for the non-pure screw segments on the κ^{th} slip system as

$$\sqrt{\overline{\boldsymbol{F}^\kappa_{ns} \cdot \boldsymbol{F}^\kappa_{ns}}} \quad \approx \quad \sqrt{\overline{\chi^\kappa_{ns}\left[\tau^\kappa\left(\bar{\boldsymbol{S}}\right)\right]^2}} \quad = \quad \varphi^\kappa\left(\bar{\boldsymbol{S}}\right).$$

But, since $\boldsymbol{m}^\kappa$ and $\boldsymbol{n}^\kappa$ do not vary in the averaging volume,

$$\varphi^\kappa\left(\bar{\boldsymbol{S}}\right) = \left|\tau^\kappa\left(\bar{\boldsymbol{S}}\right)\right| \sqrt{\overline{\chi^\kappa_{ns}}}.$$

It appears that yielding for the pure screw segments cannot be subsumed under a slip system formalism even for the single crystal case (e.g. consider the case of two slip systems that share the Burgers vector of the screw and have equal resolved shear stress on them), and a separate yield function of the form

$$\varphi_{ps}\left(\bar{\boldsymbol{S}}\right) = \sqrt{\bar{\boldsymbol{S}}\,\bar{\boldsymbol{S}}^T : \overline{\chi_{ps}\boldsymbol{m} \otimes \boldsymbol{m}} \; - \; \bar{\boldsymbol{S}} : \overline{\left[\chi_{ps}\left(\boldsymbol{m} \otimes \boldsymbol{m}\right) \otimes \left(\boldsymbol{m} \otimes \boldsymbol{m}\right)\right]} : \bar{\boldsymbol{S}}}$$

is mandated.

For the plastic flow corresponding to the κ^{th} slip system, consider the averaged plastic strain rate produced by non pure-screw segments on the system κ, under the mean field assumption on the stress:

$$\begin{aligned} \boldsymbol{L}^p_\kappa \; &:= \; \overline{\chi^\kappa_{ns}\left\{\boldsymbol{\alpha} \times \boldsymbol{V}\right\}\left(\bar{\boldsymbol{S}}\right)} \; = \; \overline{\chi^\kappa_{ns}\left(\rho \boldsymbol{m} \otimes \boldsymbol{l}\right) \times \boldsymbol{F}^\kappa_{ns}} \; = \; \overline{\chi^\kappa_{ns}\frac{|\alpha|}{B}\left(\boldsymbol{m}^\kappa \otimes \boldsymbol{l}\right) \times \left(\tau^\kappa\left(\bar{\boldsymbol{S}}\right)\boldsymbol{n}^\kappa \times \boldsymbol{l}\right)} \\ &= \overline{\chi^\kappa_{ns}\frac{|\alpha|}{B}}\; \tau^\kappa\left(\bar{\boldsymbol{S}}\right)\; \boldsymbol{m}^\kappa \otimes \boldsymbol{n}^\kappa, \end{aligned}$$

following (9). It follows that

$$\frac{\partial \varphi^{\kappa}}{\partial \bar{\boldsymbol{S}}} // \left(\boldsymbol{L}^{p}_{\kappa}\right)_{sym}.$$

Following the considerations of the previous section (14), the average plastic strain rate produced by the pure screw segments in the averaging volume may be approximated by $\boldsymbol{L}^{p}_{ps}$ defined by

$$\boldsymbol{P}_{ps} := \chi_{ps} \boldsymbol{m} \otimes \boldsymbol{m} \bar{\boldsymbol{S}} - \left[\chi_{ps} (\boldsymbol{m} \otimes \boldsymbol{m}) \otimes (\boldsymbol{m} \otimes \boldsymbol{m})\right] : \bar{\boldsymbol{S}}$$

$$\boldsymbol{L}^{p}_{ps} \approx \overline{\chi_{ps} \boldsymbol{\alpha} \times \boldsymbol{V}\left(\bar{\boldsymbol{S}}\right)} = \left(\overline{\frac{\chi_{ps} |\boldsymbol{\alpha}|}{B}}\right) \bar{\boldsymbol{P}}_{ps} + \overline{\left\{\frac{\chi_{ps} |\boldsymbol{\alpha}|}{B} - \left(\overline{\frac{\chi_{ps} |\boldsymbol{\alpha}|}{B}}\right)\right\} \boldsymbol{P}_{ps}}$$

so that

$$\frac{\partial \varphi_{ps}}{\partial \bar{\boldsymbol{S}}} // \left(\boldsymbol{L}^{p}_{ps}\right)^{red}_{sym} \quad ; \quad \left(\boldsymbol{L}^{p}_{ps}\right)^{red} := \left(\overline{\frac{\chi_{ps} |\boldsymbol{\alpha}|}{B}}\right) \bar{\boldsymbol{P}}_{ps}.$$

Thus, if we define a single crystal model by the *plastic flow*

$$\boldsymbol{L}^{p}_{red} := \sum_{\kappa} \boldsymbol{L}^{p}_{\kappa} + \left(\boldsymbol{L}^{p}_{ps}\right)^{red}$$

and $K + 1$ yield functions

$$\varphi^{\kappa}\left(\bar{\boldsymbol{S}}\right), \varphi_{ps}\left(\bar{\boldsymbol{S}}\right),$$

where K is the total number of slip systems in the crystal, then the model displays associated flow. To display the similarity (and difference) of the model with conventional single crystal plasticity theory, we define

$$\dot{\gamma}^{\kappa} := \overline{\chi^{\kappa}_{ns} \frac{|\boldsymbol{\alpha}|}{B}} \tau^{\kappa}\left(\bar{\boldsymbol{S}}\right) \quad ; \quad \dot{\gamma}_{ps} := \left(\overline{\frac{\chi_{ps} |\boldsymbol{\alpha}|}{B}}\right) \left|\bar{\boldsymbol{S}}\right|$$

and write

$$\boldsymbol{L}^{p}_{red} := \sum_{\kappa} \dot{\gamma}^{\kappa} \boldsymbol{m}^{\kappa} \otimes \boldsymbol{n}^{\kappa} + \frac{\dot{\gamma}_{ps}}{\left|\bar{\boldsymbol{S}}\right|} \bar{\boldsymbol{P}}_{ps}.$$

The model incorporates plastic spin, of course. Interestingly, for materials dominated by pure screw dislocations (as happens in the case of some bcc materials), the model would seem to predict different response compared to conventional crystal plasticity theory. We note here that the level of detail of the underlying microscopic theory considered herein is not sufficient to deal with the non-Schmid behaviors arising from screw dislocation core effects in some BCC metals or intermetallics [8].

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